NEW YORK UNIVERSITY
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# A SELF-CONSISTENT CALCULATION OF THE DISSOCIATION OF OXYGEN IN THE UPPER ATMOSPHERE

## PART II: THREE-BODY RECOMBINATIONS

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## Abstract


The dissociation region of oxygen molecules is treated in the same "self-consistent" manner described in a previous paper[1,2], except that now the densities of atomic and molecular oxygen have been calculated as functions of the altitude, on the assumption that the main recombination process between oxygen atoms is a three-body non-radiative process. The result of the present work indicates that dissociation occurs at an altitude about 5 Km higher than the corresponding altitude of reference 1. Furthermore, the region of dissociation is broader than in the model of reference 1. The maximum atomic density is $0.5 - 1 \times 10^{13}/\ cm^3$.

## I. Introduction

In two previous papers[1,2] the densities of atomic and molecular oxygen in the upper atmosphere were calculated in terms of two different models. Both of these models were carried out in a "self-consistent" manner, that is, no a-priori assumptions were made as to the distribution of molecular or atomic oxygen. (Such assumptions have been made by previous authors in the field, as was pointed out in references 1 and 2).

In the first model it was possible to calculate the distribution of temperature as well as the distribution of the atomic and the molecular oxygen densities. In the second model, a temperature distribution was assumed in order to avoid the necessity of imposing a severe assumption, used in the first model, with respect to energy balance.

In both of these models the principal recombination process was assumed to be a two-body radiation process. The present paper is to be regarded as a direct extension of reference 2; the assumption of two-body recombinations is replaced by the assumption that the oxygen atoms recombine in a three-body process. Therefore instead of repeating the various details of the model of reference 2 and of the method of solution of the equations for the densities, we shall merely indicate the modifications.

## II. The Three-Body Recombination Process

The principal modification of reference 2 which we introduce in the present work is to replace the two-body recombination process (11) there by the three-body recombination process (10). The rate of recombination of the oxygen atoms is taken to be $Cn_M n_p^2$ where C is the three-body recombination coefficient and $n_M$ is the number density of the third body M. Various additional assumptions are now necessary, since the recombination coefficient C and the number density $n_M$ are not known. First of all

we shall assume that all atoms or molecules are equally efficient as third bodies. Once one makes this assumption it is clear that it is sufficient to take $n_M$ as the number density of nitrogen molecules, since nitrogen predominates so greatly in the region of interest. We further assume that it obeys its own barometric equation of the usual exponential type when the temperature is taken as constant. We have prescribed that just below the altitude at which dissociation becomes important, the number density of nitrogen molecules will be four times that of oxygen, that is, the oxygen-nitrogen ratio is the same as at sea-level.

For C we have taken two values, namely $C = 10^{-32}$ and $C = 2 \times 10^{-33}$. These are typical values given by chemists for three-body processes and used by previous workers on the present problem (see e.g. reference 3).

The formulas and method of procedure are substantially the same as those of reference 2. We need merely replace the two-body recombination coefficient B' by

$$B' = Cn_M$$

where $n_M$ is a function of the altitude and is given by the barometric equation as described above. (Incidentally there is a misprint in reference 2. The letter B in equations (15) through (17) should be replaced by B'.)

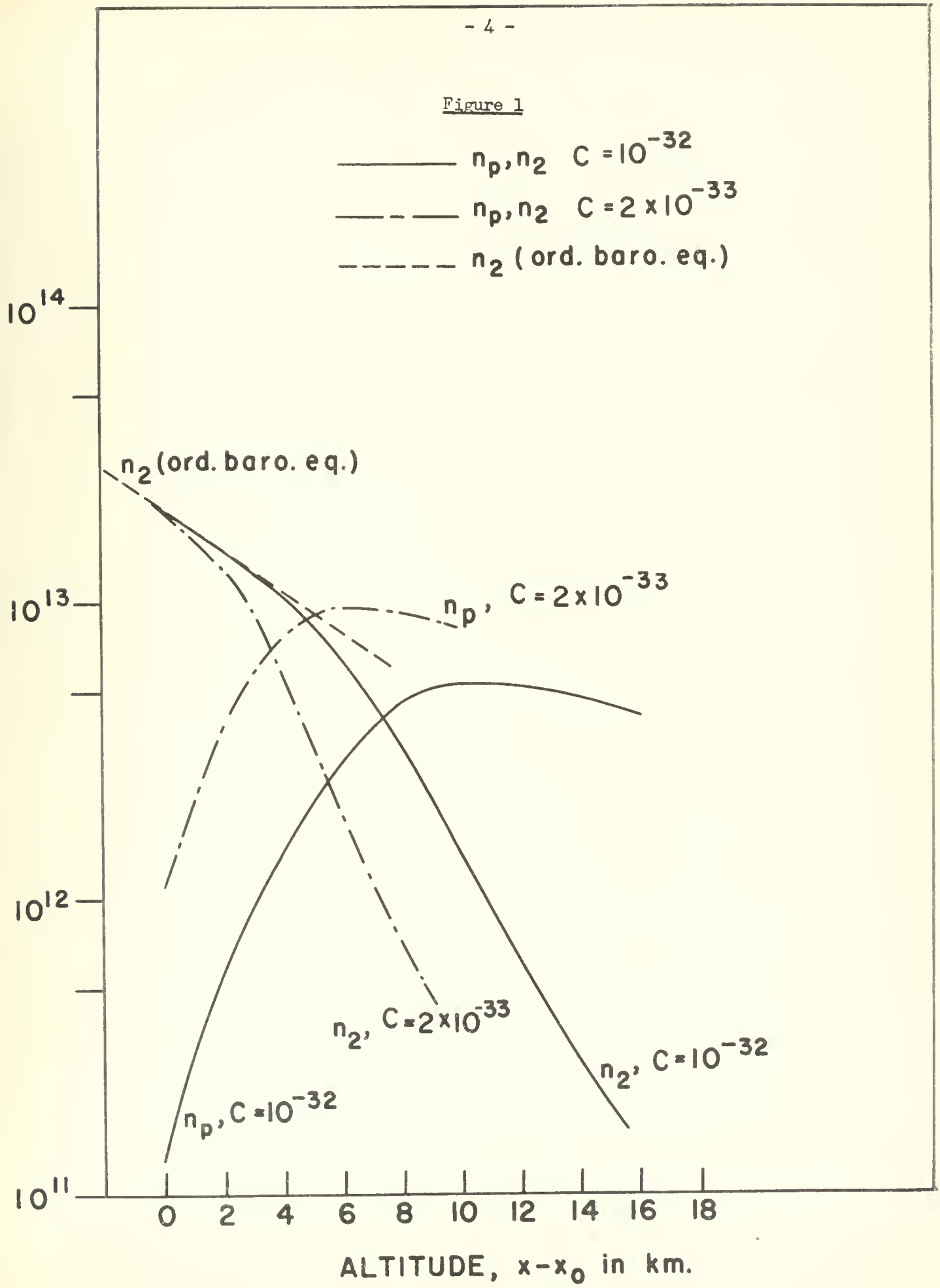
## III. Results

The results of the calculation are summarized in Figure 1. The temperature was taken as $300^\circ$ K. The altitude $x_o$ was chosen to correspond to the value $n_2 = 2 \times 10^{13}/\text{cm.}^3$. Only above this altitude does dissociation become important. If we use the pressure vs. altitude results of reference 4, we find that $x_o$ is about 90 Km. The graphs of $n_2$ and $n_p$ are given in Figure 1. We have also superposed the graph of $n_2$ as it would be if no dissociation took place - the values are obtained from the ordinary barometric equation.

It is seen that in the present model dissociation occurs at higher altitudes (about 5 Km. higher) than in the model of reference 2. This result is a consequence of the use in this paper of a greater value for the effective two-body recombination cross-section $Cn_M$. Hence in the present model the oxygen atoms can recombine more readily than in the model of reference 2 and only at higher altitudes are dissociations numerous enough to ensure number balance. Another striking difference between the present results and those of reference 2 is the broadness of the region in which dissociation takes place - about 25 Km., as opposed to less than 15 Km. of reference 2.

These differences between the results of the present paper and those of reference 2 (and reference 1) indicate the high degree of sensitivity of the results to the model used. We must conclude that the problem of obtaining really useful numerical results for the dissociation of oxygen cannot be solved until much more reliable data on the various cross-sections is available; then it will be clear which model should be used. This result, though not surprising, indicates that any numerical results which are available at present must be accepted only with great reserve.

Figure 1


$n_p, n_2$ $C = 10^{-32}$
$n_p, n_2$ $C = 2 \times 10^{-33}$
$n_2$ (ord. baro. eq.)
$10^{14}$
$10^{13}$
$10^{12}$
$10^{11}$
$n_2$ (ord. baro. eq.)
$n_p$, $C = 2 \times 10^{-33}$
$n_2$, $C = 2 \times 10^{-33}$
$n_2$, $C = 10^{-32}$
$n_p$, $C = 10^{-32}$
0 2 4 6 8 10 12 14 16 18
ALTITUDE, $x - x_0$ in km.

## References

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4. The Rocker Panel, Phys. Rev. 88, 1027 (1952).